First-principles modeling for optimization of process operations

Costas Pantelides
FOCAPO/CPC, January 9th, 2017
Outline

- First-principles process modelling
- Optimization of process operations
  - beyond the single plant boundary
- Model-based process monitoring
- First-principles modeling for model-based automation
- Concluding remarks
First-principles modeling

- Few, if any, models are really “first principles”

- Key differentiator is use of prior knowledge
  - not (just) measurements from the specific system under consideration

- Questions that matter in the real world
  1. Does the model predict the effects of external controls and disturbances on the process KPIs?
     - within the accuracy required by the business objectives
  2. Are the required computations feasible and tractable?
  3. What is the cost of developing & maintaining the model?
Dimensions of process modeling

Model detail
- 4d+
- 3d
- 2d
- 1d
- Lumped

Model scope
- Concept
- FEED
- Equipment design
- Detail engineering
- Operations
- Particle
- Sub-unit
- Unit
- Plant
- Supply chain
- Product function

Model application

© 2017 Process Systems Enterprise Limited
Current drivers for process modeling

Use validated models that are predictive over wide ranges of design & operating parameters

→ increase reliability/reduce risk in model-based decisions

Leverage modeling investment across process lifecycle

→ reduce cost of model development & maintenance

Capture all important interactions

→ formulate meaningful engineering objectives
Optimization of process operations
Beyond the single plant boundaries
Priorities in process optimization

- #1 Realisability/feasibility  →  Model fidelity
- #2 Robustness  →  Ability to obtain feasible points of large sets of nonlinear equality constraints
- #3 Efficiency  →  Execution within required timeframe
- #4 Quality of solution  →  Effective exploration of decision space Global optimality
Integrated gas production & processing networks
Basrah Gas Company

~20 mmSCM/d of gas (170,000 boe/d)
- significant flaring

D. Aluma, N. Thijssen, K.M. Nauta, C.C Pantelides, N. Shah
“Optimize an integrated natural gas production and distribution network”
Integrated gas production & processing network
4 fields + 2 processing facilities + connecting pipelines
Operational optimization objectives

- **PROFITABILITY**
  - Given tight market conditions, small improvements in the supply chain and operating conditions could be critical to business viability

- **RELIABILITY**
  - Satisfy customers
  - Honour contractual delivery commitments
    - e.g. under conditions of field decline or equipment failure

- **FLARE REDUCTION**
  - Severe environmental and economic penalties for inefficient operation
Integrated gas production & processing network
Top-level model

North Rumaila
West Qurna
North Rumaila NGL
~300k NLAES
KAZ NGL & LPG
Um Qasr Storage & Marine Terminal
South Rumaila
Zubair
Integrated gas production & processing network
Second-level models

Compressor Stations
(n trains)

NGL plant

LPG plant

Pipelines

Distributed model
Haaland Correlation
Heat transfer
Operational optimization of integrated gas networks
Objectives, decisions & constraints

- **Normal operation**
  - Maximize profit
  - Maximize total production
  - Maximize yields of specific products
  - Minimize flaring

- **Abnormal operation**
  - Maximize production under equipment failure scenario
  - Maximize production under field decline scenario

---

### Decision Variables

<table>
<thead>
<tr>
<th>Decision Variables</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed gas rates from oil production</td>
<td>55</td>
</tr>
<tr>
<td>Gas-to-NGL plant splits</td>
<td>4</td>
</tr>
<tr>
<td>Column reflux ratios</td>
<td>9</td>
</tr>
<tr>
<td>Column boil-up ratios</td>
<td>9</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td><strong>77</strong></td>
</tr>
</tbody>
</table>

---

### Constraints

<table>
<thead>
<tr>
<th>Constraints</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compressor duty</td>
<td>20</td>
</tr>
<tr>
<td>Column max flooding velocity</td>
<td>9</td>
</tr>
<tr>
<td>Product specifications</td>
<td>3</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td><strong>32</strong></td>
</tr>
</tbody>
</table>
## Normal operational scenarios

<table>
<thead>
<tr>
<th>Objective</th>
<th>Base Value</th>
<th>Optimal value</th>
<th>Δ %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max profitability</td>
<td>$/yr</td>
<td><em>not disclosed</em></td>
<td>+ 4.9%</td>
</tr>
<tr>
<td>Max total production</td>
<td>kg/s</td>
<td>346.9</td>
<td>359.2</td>
</tr>
<tr>
<td>Max propane yield</td>
<td>kg/kg</td>
<td>0.23</td>
<td>0.34</td>
</tr>
<tr>
<td>Min flaring</td>
<td>kg/s</td>
<td>9.85</td>
<td>1.26</td>
</tr>
</tbody>
</table>

## Abnormal operational scenarios

<table>
<thead>
<tr>
<th>Objective</th>
<th>Base Value</th>
<th>Optimal value</th>
<th>Δ %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max production under equipment failure (one KAZ NGL train down)</td>
<td>kg/s</td>
<td>233.5</td>
<td>295.3</td>
</tr>
<tr>
<td>Max production under field decline</td>
<td>kg/s</td>
<td>230.5</td>
<td>343.2</td>
</tr>
</tbody>
</table>
Operational optimization of large process systems

Summary

Take account of all system interactions & degrees of freedom

Network-wide rigorous optimization using “first-principles” models

Ensure that optimal solution satisfies all system constraints

⇒ implementable in practice without excessive “safety margins”

Explore full decision space effectively & efficiently
Model-based process monitoring
Model-based automation

Operational optimization in olefins plants

1. Cracking furnace
   - Online yield accounting and monitoring of coking

2. C2 & C3 hydrogenation
   - Detailed analysis for yield improvement

3. Refrigeration & compression

4. Whole-plant optimization
   - Offline production optimization
   - Multi-period optimization
   - Multi-site optimization
Ethylene/propylene yields essential information for good control

Difficult to get reliable exit composition data
- can only be taken some way downstream because of high temperatures
- light olefins dissolve in condensed steam
- instruments often faulty or out of service
Cracking furnace operation: coking

- Coking
  - coke deposits along length of coil
  - can be exacerbated by fluctuations in feed flowrate, steam, etc.

- Effects increase over time
  - reduced heat transfer
  - higher metal skin temperature
  - increasing pressure drop

- Lower efficiency, more energy required
- Loss of yield, shortened run length
- Potential coil damage & downtime

Key variables

- TMT: Tube Metal Temp
- CIT: Coil Inlet Temp
- COP: Coil Outlet Pressure
- COT: Coil Outlet Temp

Coke formation on tube inside wall
Model-based operations support for cracking furnaces

Online Model-based Application

- Reconciled data
  - Product yields, key temperatures, other KPIs
  - Current state of coking

- Online and offline optimization and decision support based on up-to-date model
- Accurate, up-to-date, continuous yield information based on current coking state

- Whole olefin plant optimization
- Furnace operations decision support
- Cracking furnace control
- Monitoring & diagnosis

© 2017 Process Systems Enterprise Limited
Model-based operations support for cracking furnaces

Approach 1 – simulation

■ Approach
  - Simulate over run length from known starting point – e.g. clean coil
  - Use measured values as model input variables

■ Advantages
  - Relatively simple to implement
  - Uses easily-available information e.g. $F_{in}(t)$, $x_{in}(t)$, COP(t), CIT(t), ...

■ Disadvantages
  - Assumes ‘perfect model’
  - Assumes perfect input measurements
  - Does not take advantage of redundant measurements
  - Drifts from reality over run length
Model-based operations support for cracking furnaces

Approach 2 – state estimation

- **Concept**
  - Use all available plant measurements
  - Exploit data redundancy
  - Use Bayesian approach to reconcile
    - Measurement error
    - Model error

- **Algorithms**
  - Extended Kalman Filter
  - Unscented Kalman Filter
  - Ensemble Kalman Filter
  - Particle Filtering
  - Moving Horizon Estimation

- **Challenge:** correct characterization & quantification of model uncertainty
  - Requires good understanding of physical system

Classical ODE formulation:

\[
\frac{dx}{dt} = f(x) \quad | \quad x(0) = x_0
\]

**In principle,** (almost all) index-1 DAE systems

\[
f(x, \dot{x}, z) = 0 \quad | \quad C(x(0), \dot{x}(0), z(0)) = 0
\]

are equivalent to standard ODE form

⇒ standard theory may be applied

**In practice,** coming up with reasonable estimates for matrices \( W, W_0 \) is often (very) problematic
Model-based operations support for cracking furnaces
Approach 2 – state estimation

- **Concept**
  - use all available plant measurements
  - exploit data redundancy
  - Use Bayesian approach to reconcile
    - measurement error
    - model error

- **Algorithms**
  - Extended Kalman Filter
  - Unscented Kalman Filter
  - Ensemble Kalman Filter
  - Particle Filtering
  - Moving Horizon Estimation

- **Challenge:** correct characterization & quantification of model uncertainty
  - requires good understanding of physical system

**Derive filters directly from DAE/PDAE form:**

\[
\begin{align*}
  f(x, \dot{x}, z, u + w, \theta + \omega) &= 0 \\
  C(x(0), \dot{x}(0), z(0), u(0) + w_o, \theta + \omega) &= 0 \\
  w &\sim (0, W), \quad \omega &\sim (0, \Omega), \\
  w_o &\sim (0, W_o)
\end{align*}
\]

**From off-line parameter estimation**
Model-based operations support for cracking furnaces

Approach 2 – state estimation

- Concept
  - use all available plant measurements
  - exploit data redundancy
  - Use Bayesian approach to reconcile
    - measurement error
    - model error

- Algorithms
  - Extended Kalman Filter
  - Unscented Kalman Filter
  - Ensemble Kalman Filter
  - Particle Filtering
  - Moving Horizon Estimation

- Challenge: correct characterization & quantification of model uncertainty
  - requires good understanding of physical system

Subset of parameters may drift over time:

\[
\frac{d\bar{\theta}}{dt} = 0, \quad \bar{\theta}(0) = \theta + \omega_o
\]

⇒ online model recalibration

N.B. Apply only where physically justified

Coking rate:

\[
r_{coking}(z) = k_{c1}c_{C_2H_6}(z) + k_{c2}\left(\frac{c_{C_2H_6}^2}{c_{C_3H_8}}\right) + k_{c3}c_{C_3H_6} + k_{c4}c_{1-3but.}
\]
Model-based operations support for cracking furnaces

Approach 2 – state estimation

Control inputs
(no/little uncertainty)
\( F_{in}(t), x_{in}(t) \)
\( F_s(t) \)
\( COP(t) \)
\( CIT(t) \)

Plant measurements
(significant uncertainty)
\( \Delta P(t) \)
\( CST(t) \)
\( TMT(t) \)
\( x_{\text{ethane}}(t) \)

Optimal KPI estimates
Yields (t)
\( \Delta P(t) \)
\( TMT(t) \)
Coke thickness \((z,t)\)
\( \text{COT}(t) \)
Fuel Consumption (t)

Extended Karman Filter

- DAE model size
  - Differential variables 260
  - Algebraic variables 44,240
- Parameters recalibrated 6
- Measurements \(~120\)
- Sampling frequency 60 s

Typical results

Ethylene in product (kg/kg)

Total coke deposition (kg)
Real-time monitoring of olefins cracking furnaces

Summary

Moderately large models within scope of current computational capability (but careful problem formulation is necessary)

Good characterization of coking kinetics (difficult to achieve otherwise)

Real-time monitoring using self-calibrating "first-principles" models

- Accurate estimates of product yields
- Accurate estimates of cracking furnace coking
- Correct basis for whole-plant optimization
- Early detection of abnormal coking rates
- Updating of MPC model

⇒ derive full benefit from investment in Advanced Process Control
First-principles modeling for model-based automation
Model-based automation

Plant Data

Data conditioning

State estimation/Online model re-calibration

Up-to-date (re-calibrated) model

Current plant state

Plant

Regulatory Control System

Set-point/trajectory optimization

MPC model derivation

Economic MPC

Decision support via future scenario simulation

Monitoring & diagnosis

Model Predictive Control (Linear / Nonlinear)

Optimal CV set-points/trajectories

Reduced/linear model(s)

Unmeasured CVs

© 2017 Process Systems Enterprise Limited
First-principles modeling for model-based automation

- Model construction
  - Relatively easy

- Model validation
  - Usually the rate-determining step

- Model configuration for online deployment

Up-to-date (re-calibrated) model
Model-based automation for spray-drying systems

Model construction
Model-based automation for spray-drying systems

Model validation

Dynamic vapour sorption experiments + Adsorption isotherm model → Validated thermodynamic model

Acoustic levitation device + Single droplet drying model → Validated kinetic model

Spray dryer experiments + Spray dryer model → Validated spray dryer model

Requires significantly less API than statistical approach; thermodynamic and kinetic models are equipment-independent.
Model-based automation for spray-drying systems
Potential benefits of first-principles approach

- Initial implementation requires less experimentation/API amount effort than traditional approaches
- Implementation on another plant for the same material allows reuse of thermodynamic and kinetic model → reduced model validation effort
  - supports tech transfer in pharma
- Implementation on same plant for another material allows reuse of residence time part of process model → reduced model validation effort
  - particularly relevant to food and consumer goods sectors
Concluding remarks
Current drivers for process modeling

- Use validated models that are predictive over wide ranges of design & operating parameters
  ➔ increase reliability/reduce risk in model-based decisions

- Capture all important interactions
  ➔ formulate meaningful engineering objectives

- Leverage modeling investment across process lifecycle
  ➔ reduce cost of model development & maintenance
Current drivers for process modeling

Capture all important interactions
- formulate meaningful engineering objectives

Use validated models that are predictive over wide ranges of design & operating parameters
- increase reliability/reduce risk in model-based decisions

Leverage modeling investment across process lifecycle
- reduce cost of model development & maintenance

...will become increasingly pressing

PREDICTION:
“First-principles” models will play the dominant role in satisfying these requirements

Process modeling technology will need to handle
1. much more complex models
   - system-level complexity
   - component-level complexity
2. much wider range of applications
   - stronger support for model re-usability